

IDEAS-Watersheds Project

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IDEAS
WATERSHEDS

Accelerating watershed science through a community-driven software ecosystem

Water resources are critically important for energy production, drinking water, agriculture, and ecosystem health, but they are under increasing pressure from growing demand, land-use change, and Earth system change. Stresses on the water supply are largely transmitted through the nation's watersheds. To enable a robust, predictive understanding of how watersheds function and respond to perturbations as integrated hydro-biogeochemical systems, researchers are working to overcome challenges in multiscale and multiphysics modeling. At the same time, disruptive changes in computer architectures are creating significant uncertainty in programming models. This convergence of interdisciplinary challenges drives the Interoperable Design of Extreme-scale Application Software (IDEAS) family of projects to provide community-based approaches to software development. Within this family, the IDEAS-Watersheds project seeks to enhance scientific productivity through an agile approach centered on adapting modern software engineering tools, practices, and processes to build a flexible scientific software ecosystem. As part of the Environmental System Science (ESS) program within the U.S. Department of Energy's (DOE) Office of Biological and Environmental Research (BER), the IDEAS-Watersheds project is helping to advance systems-level understanding of how watersheds function and to translate that understanding into advanced, science-based models of watershed systems.



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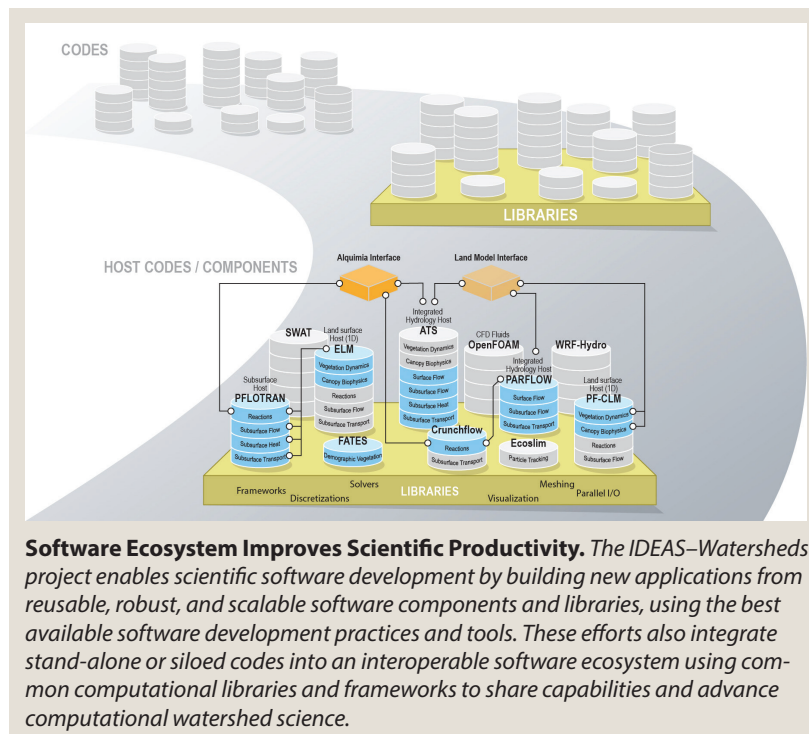
Research Activities

IDEAS-Watersheds is organized around six research activities—three partnership activities and three crosscutting activities—to address important scientific challenges and advance software development methodologies and engagement in the growing community-driven software ecosystem.

Partnership Research Activities

Each partnership activity is undertaken jointly with one of ESS's interdisciplinary Science Focus Areas (SFAs) at Lawrence Berkeley National Laboratory (LBNL), Oak Ridge National Laboratory (ORNL), and Pacific Northwest National Laboratory (PNNL). These activities address biogeochemical cycling in streams across a wide range of stream orders in disparate climates and land-use conditions.

LBNL Watershed Function SFA. Perturbations to mountainous watersheds (e.g., floods, drought, and early snowmelt) affect the downstream delivery of water, nutrients, carbon, and trace metals.



Software Ecosystem Improves Scientific Productivity. The IDEAS-Watersheds project enables scientific software development by building new applications from reusable, robust, and scalable software components and libraries, using the best available software development practices and tools. These efforts also integrate stand-alone or siloed codes into an interoperable software ecosystem using common computational libraries and frameworks to share capabilities and advance computational watershed science.

Currently, no single model can capture all the relevant processes across this domain at fine resolution. The partnership activity with the LBNL SFA aims to develop a multiscale modeling framework that enables consideration of processes at different resolutions within the watershed, including the software tools and workflows required for this framework.

ORNL Critical Interfaces SFA. Metabolically active transient storage zones (MATSZs) are biogeochemical hotspots or regions surrounding stream channels where downstream water movement is delayed. The partnership activity with the ORNL SFA is developing a stream corridor modeling framework that allows laboratory-derived understanding of biogeochemical processes occurring in slow-flowing MATSZs to be combined with reach-scale observations. The partnership supports the overarching strategy of developing a multiscale river network modeling system to represent how MATSZs influence stream biogeochemistry and, ultimately, downstream water quality by processing significant portions of carbon, nutrients, and trace metals.

PNNL River Corridor SFA. River corridor science is conducted in the context of larger watershed processes that define boundary fluxes and exert other controls on hydrological exchange. These controls include interactions among variable river surface elevation ("stage"), hydromorphic setting, and hydrogeological heterogeneity. To determine how these processes and interactions influence river corridor hydro-biogeochemical function, models must include land-surface and

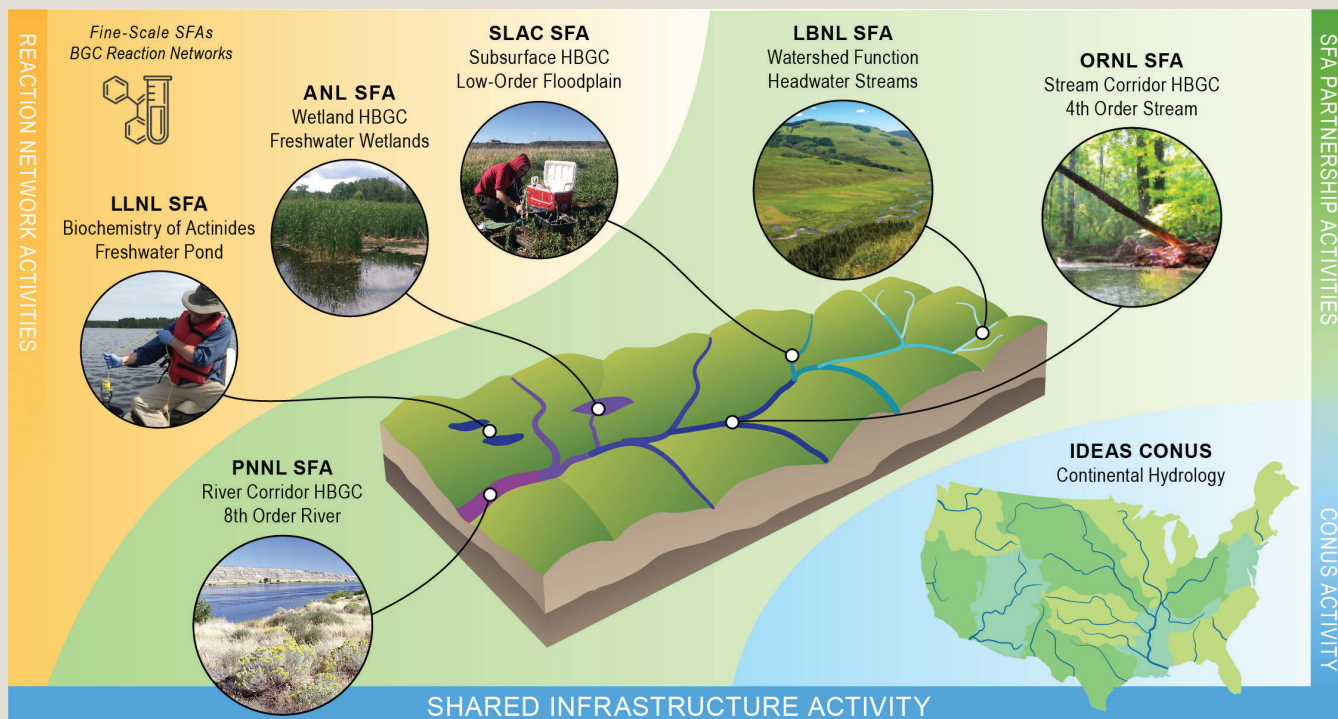


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IDEAS-Watersheds Project. Research activities address the needs identified in project partnerships along three cornerstones of watershed research—reaction networks, watershed hydro-biogeochemistry (HBGC), and continental hydrology—while enabling the development of shared solutions to move information and capability across the project and ESS as a whole.

groundwater processes over domains much larger than the river corridor itself. The partnership activity with the PNNL SFA aims to enable fundamental understanding of the hydro-biogeochemical function of dynamic river corridor ecosystems and translate that understanding into predictive, interoperable models across watersheds.

Crosscutting Research Activities

Continental United States (CONUS) Activity. Simulating integrated flow over continental scales at so-called hyper-resolution is a grand challenge in computational hydrology. To adequately capture feedbacks among deeper subsurface flow, the land energy budget, and the lower atmosphere, explicit connections must be made between these systems in large-scale models. The CONUS activity supports development of an integrated hydrological modeling platform of CONUS using the ParFlow-Community Land Model (PF-CLM). The CONUS model bridges across IDEAS-Watersheds study areas and provides a scaling framework from the reach scale up to watershed and regional systems.

Reaction Network Activity. Reaction networks to describe biogeochemical transformations are a central component of ESS watershed sciences research. This activity bridges across the SFAs and develops process-explicit reaction models for aqueous complexation, surface complexation, mineral dissolution-precipitation, microbially mediated reactions, microbial dynamics, and similar processes.

Shared Infrastructure Activity. This activity coordinates development of the shared computational infrastructure. Work includes creating and advancing existing, multiscale workflow tools and software interfaces. These interfaces enable and support transfer of information across scales, customized meshing, integration of models and data, coupling of multiple process-based codes, and code interoperability.

Scientific and Community Impact

The IDEAS-Watersheds project has made significant progress in developing a flexible scientific software ecosystem to accelerate scientific

discovery and understanding in environmental systems, including completion of open-source licensing and open access to source code repositories. In addition, code teams are adopting agile methodologies and developer workflows, improving sustainability while enhancing capabilities.

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IDEAS and IDEAS-Watersheds

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